

Detailed Spectral Radiation Calculations for Nonhomogeneous Soot/Gas Mixtures Based on a Simulated Ethylene Jet Diffusion Flame

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Abstract

The purpose of this paper is to study the effects of the radiative properties of soot particles and CO_2 and H_2O gases on detailed radiative heat transfer calculations using a simulated ethylene jet diffusion flame. The YIX method is applied to calculate the radiative transfer quantities over the spectral range of 1-20 μm in a finite cylindrical enclosure with distributions for flame temperature, soot volume fraction, and gas concentrations precalculated from a modeling analysis. Scattering from soot particles is neglected. Soot only, gases only, and the combined cases are examined. The Rayleigh solution is used to calculate the absorption coefficient spectra for soot aggregates. Soot complex refractive index spectra are generated from the Drude-Lorentz dispersion model based on three frequently cited dispersion parameter sets. Results from these three dispersion parameter sets show that the difference in maximum flux divergence is 45% and that the difference in maximum radial flux is 62%. Thus current uncertainties about soot spectral refractive indices are the main limitation on accurate estimates of the radiation heat transfer from sooting combustion systems. The exponential-wide-band model is used to calculate gas absorption coefficient spectra. Generally, radiation from soot is two to three times of that from gases. Therefore both soot and gas contributions are significant, and accurate models for gas absorption coefficient spectra are crucial. More than 95% of the total gas radiation comes from the 2.73 and 4.3 μm bands of CO_2 and from the 2.67 μm bands of H_2O . The 6.3 μm H_2O band can be added to essentially account for all gas radiation, and other gas absorption bands make very little contribution. Practically, for the type of flames considered here, it is concluded that spectral contributions from beyond the 5 μm range can be neglected with less than 5% loss of accuracy in calculating the total radiative flux and its divergence.

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Nomenclature

a	=	absorption coefficient [m^{-1}]; band symmetry factor in Eq. (4)
D	=	fuel jet nozzle diameter [0.58 mm]
e	=	electron charge [$1.6022 \cdot 10^{-19}$ C]
f_v	=	soot volume fraction
g	=	damping constant of electron [sec^{-1}]
i	=	$\sqrt{-1}$
k	=	imaginary part of complex refractive index
\hat{m}	=	complex refractive index, $n - ik$
m_e	=	electron mass [$9.1096 \cdot 10^{-31}$ kg]
N	=	electron number density [m^{-3}]
n	=	real part of complex refractive index
\mathbf{q}	=	radiative heat flux vector [W/m^2]
q	=	radiative heat flux [W/m^2]
Re_D	=	Reynolds number (based on the nozzle diameter)
r	=	radial distance from fuel jet nozzle centerline [m]
S_c	=	mean line intensity [$\text{m}^2/\text{cm}/\text{g}$]
T	=	temperature [K]
z	=	axial distance from fuel jet nozzle exit [m]
β	=	mean line-width-spacing parameter
δ	=	absorption line spacing [cm^{-1}]
ϵ_0	=	permittivity constant in vacuum [$8.8542 \cdot 10^{-12}$ C ² /N/m ²]
η	=	wave number [cm^{-1}], $1/\lambda$
λ	=	wavelength [μm]
ρ	=	density of the gaseous mixture [kg/m^3]
σ	=	Stefan-Boltzmann constant [$5.6696 \cdot 10^{-8}$ W/m ² /K ⁴]
ω	=	resonant frequency [sec^{-1}]; bandwidth parameter in Eq. (4) [cm^{-1}]

Subscripts

c	=	free, conductive electron
i	=	bound electron
r	=	radial direction
z	=	axial direction
λ, η	=	spectral

Superscript

*	=	effective mass of free electron
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Introduction

Radiative heat transfer from a soot/gas mixture plays an important role in the analysis of hydrocarbon-fueled combustion systems. Measurements by Becker and Liang (1983) show that the amount of radiation can reach up to 75% of the total combustion energy release in acetylene diffusion flames. There is increasing interest in detailed analyses of radiation heat transfer in combustion systems (Carvalho et al., 1991; Song and Viskanta, 1987; Tong and Skocypec, 1992; Viskanta and Menguc, 1987) and in flames (Fairweather et al., 1992; Gore et al., 1992; Kaplan et al., 1994; Sivathanu et al., 1990). Such an analysis requires solving the radiative transfer equation (RTE) for nongray and nonhomogeneous media that are usually absorbing, emitting, and anisotropically-scattering. Two major issues to be addressed in such analyses are the advantages and limitations of various solution methods, and the effects of (and uncertainties caused by) the radiative properties of the medium.

Solving the RTE for a participating medium, homogeneous or otherwise, is generally a difficult task, due to the mathematical nature of the RTE (Siegel and Howell, 1992). For analyses involving most typical flames and combustion systems where the problem is described on a multi-dimensional geometry, both derivation and computation of the solution become more complex, and the calculation or modeling of total radiative transfer quantities based on spectral distributions poses another computational burden. Adding to all these complexities, the problem can become further complicated when the temperature distribution is unknown and thus the energy equation must be introduced to form a coupled system (i.e., the combined mode). As a result, earlier studies on soot/gas mixtures have been limited to a one-dimensional (1-D) geometry using an approximate solution. Yuen (1982) used the P_1 spherical harmonics approximation and a wide-band model for the gas absorption coefficient to calculate the heat flux and temperature distribution through a 1-D slab of gray-soot/nongray- CO_2 mixture under radiative equilibrium. The paper introduced the equivalent absorption coefficient concept, and showed the significant differences between gray and nongray results. Smith et al. (1987) applied the zone method for analyzing radiative and conductive transfer for a soot/gas mixture between infinite parallel plates at uniform temperatures. Using a weighted sum of the gray gases model of Felske and Charalampopoulos (1982), they showed that the soot radiation dominates the gas radiation and significantly reduces the heat transfer between plates. Thynell (1990) used an improved P_1 approximation to calculate total hemispherical emissivities of gas-soot-particle mixtures, wherein gas absorption coefficients were evaluated from the exponential-wide-band model and soot absorption coefficients were assumed inversely proportional to the wavelength. Modest and Sikka (1992) also used the P_1 approximation, but applied equivalent stepwise gray properties by utilizing the mean beam length

concept. They formulated the solution for multi-dimensional geometries, and showed that results for 1-D problems with a single-band gas and gray particles compare favorably with those from Monte Carlo calculations using the exponential-wide-band model. Yuen et al. (1992) used the zone method and the concept of absorption mean beam length to study turbulence/radiation interaction in a plane-parallel soot/gas medium. Turbulent fluctuations of temperature and gas concentration were simulated using Monte-Carlo method. They showed that time-averaged radiative properties can differ significantly from those based on mean temperature and concentrations, and that scattering effects are significant. All these studies are for homogeneous media and, in some cases, with uniform temperature, which physically may simulate such systems as a well-stirred reactor. However, these results have little applicability for and would not have revealed the complexities involved in solutions for nonhomogeneous media.

There have been studies on the radiative properties of soot/gas mixtures. Measurements of radiative intensity spectra from sooting turbulent ethylene/air diffusion flames by Gore and Faeth (1986) clearly show the significance of gas absorption bands. Several works studied the relative contributions from soot and gases in mixtures (Koçyulu and Faeth, 1993a; Lee and Tien, 1980; Viskanta and Menguc, 1987). Grosshandler and Nguyen (1985) introduced a total transmittance nonhomogeneous radiation model and the Curtis-Godson approximation (Siegel and Howell, 1992) to model methane combustion. Grosshandler and Thurlow (1991) proposed generalized state-property relations for hydrocarbon flame Planck-mean absorption coefficients.

The purpose of this paper is twofold. First, we wish to demonstrate that a recently developed YIX method for solving the radiative transfer equation for a finite cylindrical enclosure (Hsu and Ku, 1994; Hsu et al., 1992; Tan and Howell, 1990) can be applied to problems involving nongray, nonhomogeneous, absorbing, and emitting soot/gas mixtures. Second, based on results for a simulated ethylene jet diffusion flame, we address the respective contributions of absorbing gases and soot particles, and analyze the effects on radiative heat transfer quantities caused by uncertainties about radiative properties of soot particles. In this study, flame temperature, soot particle volume fraction, and CO_2 and H_2O concentration maps are precalculated from flame structure and soot formation models (Ku et al., 1995). The aspect of coupling radiation calculations with the energy equation and the flame structure solver was purposely left out so that we can focus on issues of interest, although it has been demonstrated that the coupling can be done through an iteration process with reasonably fast convergence (Ku et al., 1995). For evaluating spectral absorption coefficients, the exponential-wide-band model (Edwards, 1967) is used for gases, and the Rayleigh solution (Bohren and Huffman, 1983) is used for soot aggregates. The Drude-Lorentz dispersion model (Bohren and Huffman, 1983) is used to provide spectral refractive index

data for soot particles. The three most frequently cited spectral dispersion modeling parameter sets are used, so that comparisons among results serve to show the effects introduced by uncertainties about soot refractive index spectra. However, it is not the objective of this study to identify which dispersion model is more appropriate for radiation heat transfer calculations in flames. Scattering from soot particles, although it can be easily added, was not considered due to a lack of accurate modeling for scattering albedo and phase function. Although our current interest is in radiative heat transfer analysis for jet diffusion flames, the approach and solution scheme used in this paper can be modified to analyze other practical applications, such as fires and combustors like engines and furnaces.

Analyses

The YIX Method

The YIX method is based on the integral formulation of the radiative transfer equation in a general three-dimensional, gray, emitting, absorbing, and anisotropic scattering medium developed by Tan (1989). Crosbie and Farrell (1984) have developed similar integral expressions for the radiative intensity in a 3-D cylindrical geometry. The YIX method has been demonstrated accurate and computationally efficient both in time and storage (Hsu and Ku, 1994; Hsu et al., 1993; Tan and Howell, 1990). Details can be found in our previous paper (Hsu and Ku, 1994) about the formulation and solution scheme and about how a three-dimensional YIX solution scheme is applied to a finite cylindrical geometry for simplifying kernel calculations and for avoiding difficulties associated with treating boundary conditions. The solution is actually not limited to the axisymmetric cylindrical geometry. The solution can be easily coupled with the energy equation, since heat flux and its divergence are computed directly, for a complete heat transfer analysis and applied to complex geometries. Attempt to use the spherical harmonics (P_N) approximation for the same problem, following the work of Menguc and Viskanta (1986), failed due to seemingly numerical instabilities occurred when part of medium is in the optically thin limit.

Spectral Absorption Coefficients of Soot Particles

Flame soot particles typically exist as aggregates of small primary spherules. In visible and infrared, the size parameters of the primary spherule are usually within the range of the Rayleigh approximation (Bohren and Huffman, 1983). It has been shown that the absorption cross section of an absorbing aggregate is approximately the same as the total absorption cross section of all individual spherules (Dobbins and Megaridis, 1991; Koylu and Faeth, 1993a; Ku and Shim, 1991;

Nelson, 1989; Perry and Percival, 1986). Therefore, the absorption coefficient of soot aggregates can be calculated approximately from soot volume fraction f_v and the Rayleigh approximation as

$$a_\lambda = f_v \cdot \frac{\pi}{\lambda} \cdot \frac{36nk}{(n^2 - k^2 + 2)^2 + 4n^2k^2} , \quad (1)$$

where λ is the radiation wavelength, and n and k are the real and the imaginary parts, respectively, of the complex refractive index of soot.

The Drude-Lorentz dispersion model (Bohren and Huffman, 1983; Felske, 1983) is used to model the complex refractive index, $\hat{m} = n - ik$, of soot. This dispersion relationship is based on the complex electric displacement obtained from a classical damped oscillator model. The Lorentz interaction of bound electrons (mass m) with incident electric field (at frequency ω) is modeled as a set of linear oscillators (with a number density of N_i) each having a resonance frequency ω_i and a damping constant g_i . The Drude's model for conduction electrons is essentially the same as the bound electrons except that the resonant frequency ω_i is zero, since no restoring force exerts on the free electrons. By combining the polarization (in terms of the solved electric displacement) with the medium permittivity (ϵ) equations, the following expressions are obtained

$$n^2 - k^2 = 1 + \sum_i \frac{N_i(\omega_i^2 - \omega^2)e^2/m_e\epsilon_o}{(\omega_i^2 - \omega^2)^2 + \omega^2 g_i^2} - \frac{N_c e^2/m_e^*\epsilon_o}{(\omega^2 + g_c^2)} , \quad (2)$$

$$2nk = \sum_i \frac{N_i \omega g_i e^2/m_e\epsilon_o}{(\omega_i^2 - \omega^2)^2 + \omega^2 g_i^2} + \frac{N_c g_c e^2/m_e^*\epsilon_o}{\omega(\omega^2 + g_c^2)} . \quad (3)$$

It should be pointed out that the applicability of the Drude-Lorentz model to soot particles and the accuracy of the resulting refractive index spectra still remain to be proven (Ku, 1985). Significant spread has been observed among published soot spectral refractive index data, caused primarily by uncertainties exist in soot primary/aggregate size and morphology measurements and in scattering theories for soot aggregates (Dobbins and Megaridis, 1991; Felske et al., 1986; Ku and Shim, 1990). We apply the Drude-Lorentz model with three frequently cited modeling parameter sets and use the comparison of results to show how sensitive the radiation heat transfer calculations are to different soot refractive index spectra. These three dispersion parameter sets are listed in Table 1. As pointed out by Habib and Vervisch (1988), in comparing their parameter set to the other two, the most significant difference among three sets of parameters is the value of N_c , the free electron number density. After adjusting for differences in the effective mass of free electron, the effective N_c values from Dalzell and Sarofim (1969) and from Lee and Tien (1980)

are approximately 2 and 1 order of magnitude, respectively, greater than that of Habib and Vervisch (1988). With smaller nk value being the dominant factor in Equation (1), the absorption coefficient (actually the absorption cross section) obtained from Habib and Vervisch's parameter set is greater than those from the other two sets. Figure 1 shows the spectral absorbing coefficient calculated from three dispersion parameter sets for a volume fraction of 10^{-6} for the spectral range of 1-20 μm . It is noted that Dalzell and Sarofim's and Lee and Tien's results are relatively close to each other, especially in longer wavelengths.

Spectral Absorption Coefficient of Gas

Spectral absorption coefficients for CO_2 and H_2O gases is calculated from the exponential-wide-band model by Edwards (1976), which can be expressed as

$$a_\eta = \rho \frac{S_c}{\delta} , \quad (4)$$

where

$$\begin{aligned} \frac{S_c}{\delta} &= \frac{\alpha}{\omega} e^{-\frac{\alpha}{\omega} |\eta - \eta_c|} , \\ \alpha &= C_1 , \\ \omega &= C_3 . \end{aligned}$$

Parameters in the equation are defined in Nomenclature, with more details in Edwards (1976). Details about C_1 and C_3 and their values for several gases can be found in Siegel and Howell (1992) and Edwards (1976). Equation (4) indicates that the gas absorption coefficient depends on the temperature, pressure, and concentration. Yuen and Ma (1992) have demonstrated that this model can accurately predict the emittance data from Hottel's chart (Hottel and Sarofim, 1967) to within 10%. The approximated exponential-wide-band eliminates the need for detailed line-by-line structure (each band could contain as many as 10^4 vibration transition lines) and consequently improves the computational efficiency (Tong and Skocypec, 1992; Hsu et al., 1993).

There are several other numerical methods available for solving the radiative transfer equation involving nongray absorbing gases. The weighted sum of gray gas method (Hottel and Sarofim, 1967; Modest, 1991) is simple and computationally efficient, but not very accurate and has only been applied to homogeneous non-scattering media within black enclosures. The ultimate line-by-line calculation is obviously the other extreme. In between there are methods such as the k -distribution (Domoto, 1974; Goody and Young, 1989; Tang and Brewster, 1992), the equivalent c - k method (Domoto, 1974; Goody et al., 1989), and mapping transformation technique (West et al., 1990) which are fairly accurate, but require much more computational time. The exponential-

wide-band model seems to be the best compromise in terms of both accuracy and computational efficiency, especially when spectral integration points are optimally selected to concentrate on absorption bands.

Spectral Integration

Since the spectral variation of soot particle absorption coefficient is relatively smooth compared with that of CO₂ and H₂O, the selection of integration points is based on the spectral variation of absorption coefficient of gases. A detailed discussion of the selection of the optimal integration points and a CO₂ absorption coefficient spectrum can be found in Hsu et al. (1993). For nongray media, first the YIX distance and discrete ordinates angular quadratures are calculated at each spectral integration point, and then spectral quantities are summed up using trapezoidal rule (Hsu et al., 1992; Hsu et al., 1993).

Results and Discussions

The YIX solution developed for a finite cylindrical geometry is applied to analyze radiative heat transfer in an ethylene (C₂H₄) jet diffusion flame in quiescent air. It has a nozzle diameter of $D = 0.58$ mm and a fuel flow rate of 3.96 cm³/sec, which yields a Reynolds number of $Re_D = 536$. Figure 2 shows the contours for flame temperature, CO₂ concentration, and soot volume fraction. These are numerically calculated from flame structure and soot formation models (Ku et al., 1995). The resulting H₂O concentration contours are nearly identical to those of CO₂, as confirmed by results in Sivathanu and Faeth (1990). The computational domain for radiative transfer is between $0 \leq r/D \leq 130$ and $0 \leq z/D \leq 500$ using a 65x100 grid. The local volume fraction actually varies from as low as 10^{-20} to about 10^{-6} within the whole computational domain, whereas the local gases' concentrations change from 10^{-7} to about 10^{-1} . All boundaries are assumed to be black and at a uniform temperature of 300 K. The spectral range of interest is from 1 to 20 μ m. In Figure 2 and subsequent figures for results, only the flame core and nearby region are shown, since very little radiative heat transfer occurs beyond $r/D > 31$, due to a low medium temperature and small optical thickness.

Most calculations were performed on a Cray Y-MP/C98 supercomputer. A first YIX integration point of 0.001 and S12 discrete ordinates set for angular quadratures were used in all calculations. Although S16 was used previously for gray calculations (Hsu and Ku, 1994), a lower order discrete ordinates set is used for nongray calculations here, since the heat flux and its

divergence are dominated by optical-thick regions of the spectrum (Hsu et al., 1992; Hsu et al., 1993). The same set of integrating points is applied to all cases, even though soot only cases can be calculated with much fewer points with little or no loss of accuracy. Typical run times are less than a half-hour for soot only cases, and about 5 hours for gases only and soot/gas cases. The latter is more time-consuming because of the increased number of distance integration points within the spectral regions around gas absorption bands. A significant and linearly proportional reduction in CPU time can be obtained by further lowering the number of discrete ordinates directions, and when done properly, it should result in little or no loss in accuracy for cases involving absorbing gases. Hsu et al. (1993) showed that a factor of 7 reduction in execution time with little loss in accuracy is possible in absorbing band regions using an S4 set with 24 discrete ordinates directions as compared to 168 directions for an S12 set. Reduction in CPU time can also be expected after fine-tuning the code for vectorization. Further time savings can be achieved through parallel-processing of spectral integrations and YIX distance quadratures involving contributions from all nodes to the node of interest.

Figures 3 - 5 show results for the soot-only case based on the dispersion parameter sets of Dalzell and Sarofim (D-S), Lee and Tien (L-T), and Habib and Vervisch (H-V), respectively. Each figure consists of a contour map of normalized radiative heat flux divergence distribution on the left and a plot of normalized radial heat flux at $r/D = 31$ as a function of height on the right. The heat fluxes are normalized with respect to blackbody emissive power at 1000 K. Compared to our previous paper (Hsu and Ku, 1994), where results are based on $\hat{m} = 1.7 - i0.7$, values of the peak divergence and the maximum radial flux in this paper are nearly one order of magnitude smaller, as expected from the relative magnitudes in absorption spectrum in Figure 1. Figures 3 - 5 clearly show the strong dependence of radiative flux and its divergence on dispersion parameter sets. Among three dispersion parameter sets, H-V produces overall the largest values in both radial flux and flux divergence, L-T produces the lowest values, with D-S slightly higher than those of L-T. This is expected based on their absorption coefficient spectra in Figure 1, where H-V being the largest in the entire range and L-T the smallest in the range of 1-3 μm . Peak values in the heat flux divergence map and maximum values of radial heat flux at $r/D = 31$ are listed in Table 2. Peak flux divergence values always occur inside the flame where temperature and soot volume fraction are the highest ($r/D = 0$, $z/D \approx 155$). With the largest H-V values as a reference, the difference in maximum divergence is 45% for L-T and 41% for D-S, whereas the difference in maximum radial heat flux is 62% for L-T and 57% for D-S. These comparisons clearly show that without an accurate absorption coefficient spectrum, there could be significant uncertainties in calculations for radiation heat transfer from flame soot particles.

Figure 6 shows the results for the CO₂ and H₂O only case. As expected, the soot-only case and gases-only case each has a flux divergence contour that is very similar to that of the respective concentration contour. Consequently, distributions of flux and its divergence are significantly different between soot only and gases only cases. Figure 7 shows the results for combined soot and gases case, with H-V's soot refractive index spectrum. After examining the values for the same points in Figures 5 - 7, we confirmed that the total radiation is nearly the sum of individual contributions from soot and from gases. Table 2 also includes the peak divergence and the maximum radial heat flux for gases only and soot/gas mixture cases. Comparing the gases only case to soot/gas mixture case, the divergence at $r/D = 1$ and $z/D = 152.5$ (the peak location for cases with soot) is only 15% and the maximum radial flux is 37%. The peak divergence for gases only case is at a different location (see Table 2) and has a larger value. Therefore, both soot and gases have significant contribution to radiation heat transfer in this type of sooting diffusion flames.

Figure 8 shows the flux divergence and both radial and axial heat fluxes at $r/D = 1$ and $z/D = 152.5$, where flame temperature and soot volume fraction are at or close to their maximum. In the figure, solid curves are for the soot/gas mixture case whereas dashed curves for the soot only (H-V) case. Maximum values of these curves occur around $1.4 \mu\text{m}$, which corresponds to the peak spectral emissive power at the flame temperature range. Although the level of radiation flux is high in the range from 0.4 to $1 \mu\text{m}$, the inclusion of this part of the spectrum is not expected to change the results significantly, since it is only a narrow spectral region. As expected from their respective absorption coefficient spectrum, soot radiation is smooth over the entire spectral range, whereas CO₂ radiation peaks around those absorbing bands at 2.73 , 4.3 , 9.4 , 10.4 , and $15 \mu\text{m}$, and H₂O radiation peaks around 1.38 , 1.87 , 2.67 , and $6.3 \mu\text{m}$. The weak absorbing band of CO₂ at $2 \mu\text{m}$ was not considered in all calculations. It is noted that there is little contribution to the total radiation from the 1.38 and $1.87 \mu\text{m}$ symmetry bands of H₂O and from the 9.4 , 10.4 , and $15 \mu\text{m}$ bands of CO₂. The contribution from the $6.3 \mu\text{m}$ H₂O band is also insignificant. More than 95% of the total gas radiation comes from the 2.73 and $4.3 \mu\text{m}$ bands of CO₂ and from $2.67 \mu\text{m}$ bands of H₂O. This suggests that spectral contributions from beyond the $5 \mu\text{m}$ range can be neglected with less than 5% loss of accuracy in total radiation quantities for this type of flames.

Conclusions

The YIX method is applied to solve radiative transfer in a finite cylindrical enclosure with nonhomogeneous, nongray, emitting, and absorbing soot/gas mixture. Numerical results are obtained for radiative heat transfer within an ethylene jet diffusion flame. Contributions from soot

scattering can be easily added if accurate modeling of albedo and phase function is available. Soot only, gases only, and combined cases are examined over the spectral range of 1-20 μm . Distribution maps for flame temperature, soot volume fraction, and gases concentration are obtained numerically from flame structure and soot formation models. The Drude-Lorentz dispersion model is used to generate soot complex refractive index spectra. Soot absorption coefficient spectra are calculated from soot volume fraction and refractive indices according to the Rayleigh solution, which has been shown to be accurate for soot aggregates. Results based on three frequently cited dispersion parameter sets show that soot radiation heat transfer calculation is very sensitive to the absorption coefficient spectrum. The difference in maximum flux divergence is 45% and the difference in maximum radial flux is 62%. Thus, current uncertainties about soot spectral refractive indices are one of the major limitations in accurately estimating the radiation heat transfer from sooting flames and combustion systems. Accurate models for gas absorption coefficient spectra are also crucial, since gases contributions are significant. The exponential-wide-band model is used to calculate the gas absorption coefficient spectrum. Overall, the contribution of soot radiation is two to three times of that from gases. Consequently, both soot and gas contributions are significant. For soot particles, the radiation flux and divergence spectra are smooth. For the type of flames studied here, it seems that spectral contributions from the weak bands of CO_2 and H_2O may be neglected without significant loss in accuracy in evaluating total radiation effects. For CO_2 gas, only contributions around absorption bands at 2.73 and 4.3 μm are significant, whereas for H_2O , only 2.67 bands are important. The 6.3 μm H_2O band can be included to achieve higher degree of accuracy. Practically, spectral contributions from beyond the 5 μm range can be neglected with less than 5% loss of accuracy in total radiation quantities for this type of flame.

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Table 1 Three different dispersion parameter sets used to calculate soot refractive indices

Ref.#	N_t	N_1	N_2	N_c	g_1	g_2	g_c	ω_1	ω_2
	(10^{27} m^{-3})				$(10^{15} \text{ sec}^{-1})$			$(10^{15} \text{ sec}^{-1})$	
D-S	35.35	2.69	28.6	0.226*	6.0	7.25	6.0	1.25	7.35
L-T	48.81	4.07	44.7	0.040	5.9	5.6	1.2	1.25	7.35
H-V	20.00	1.67	18.3	0.0070	7.0	7.25	1.2	1.25	7.35

D-S: Dalzell and Sarofim (1969), L-T: Lee and Tien (1980), H-V: Habib and Vervisch (1988).

* The number has been corrected for the effective mass of conduction electrons, $N_c = 2.26 \cdot 10^{26} = 4.06 \cdot 10^{27}/18$, which was not considered in the original work.

Table 2 A comparison of the peak flux divergence and the maximum radial flux at $r/D = 31$ for 3 soot only cases, gases only case, and soot/gas case.

Cases	Peak $\nabla \cdot \bar{q}/\sigma T^4$ ($r/D = 1$, $z/D = 152.5$)	Max. $q_r/\sigma T^4$ at $r/D = 31$
Soot 1 - Dalzell & Sarofim	53.3	0.0295
Soot 2 - Lee & Tien	49.3	0.0264
Soot 3 - Habib & Vervisch	80.8	0.0577
CO ₂ + H ₂ O	14.1*	0.0370
Soot 3 + CO ₂ + H ₂ O	94.0	0.0996

* The peak for CO₂ + H₂O case is at $r/D = 7$ and $z/D = 52.5$ with a value of 20.3.

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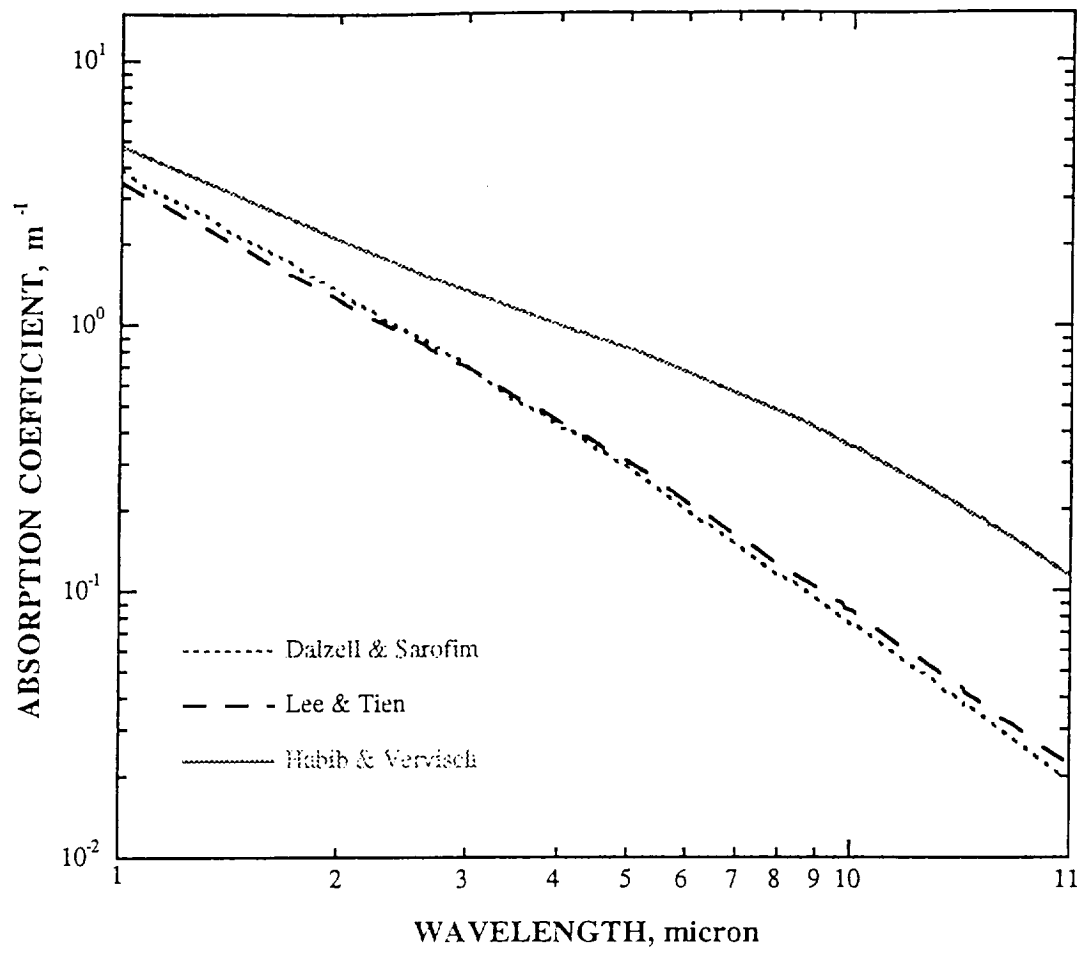


Figure 1

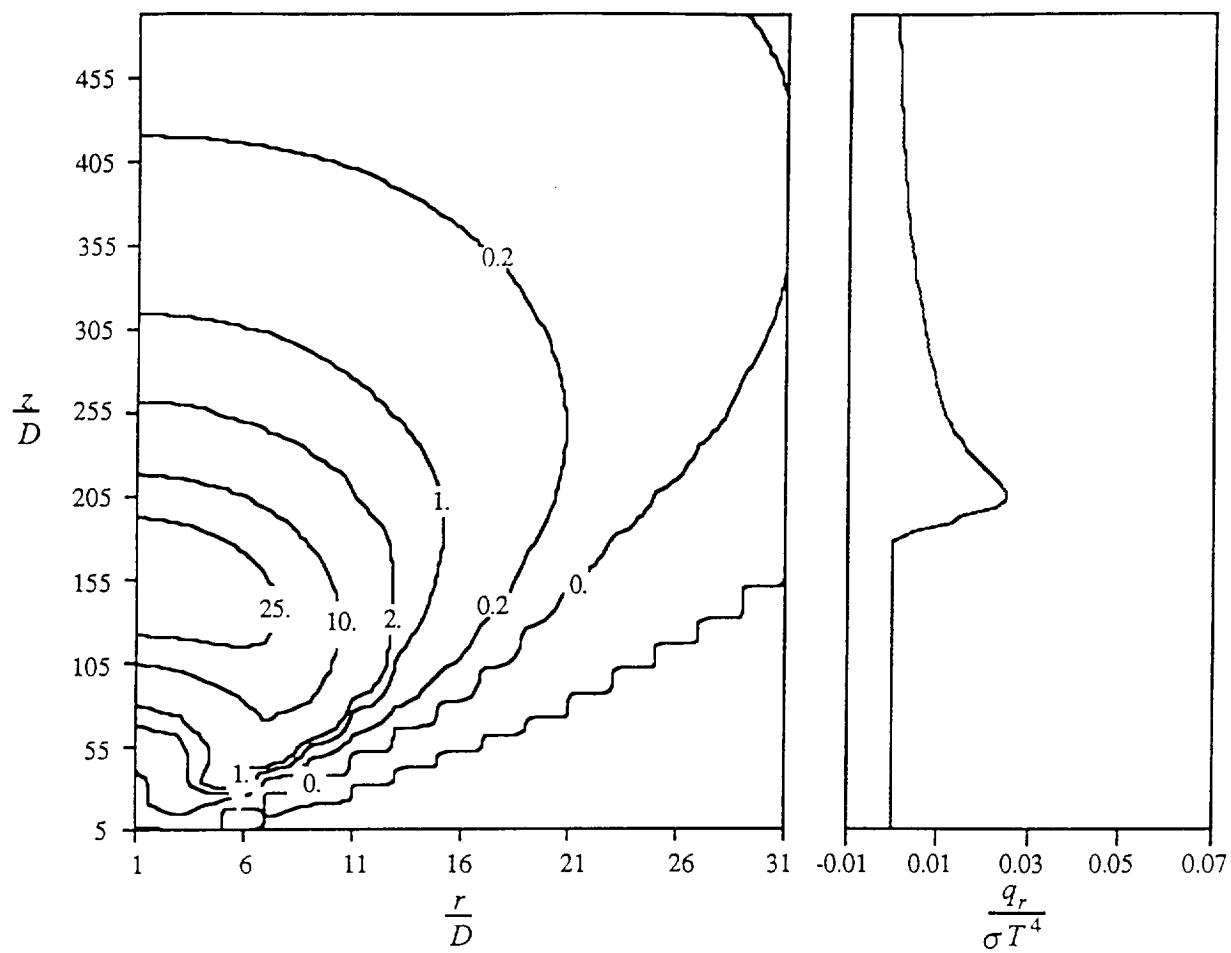


Figure 3

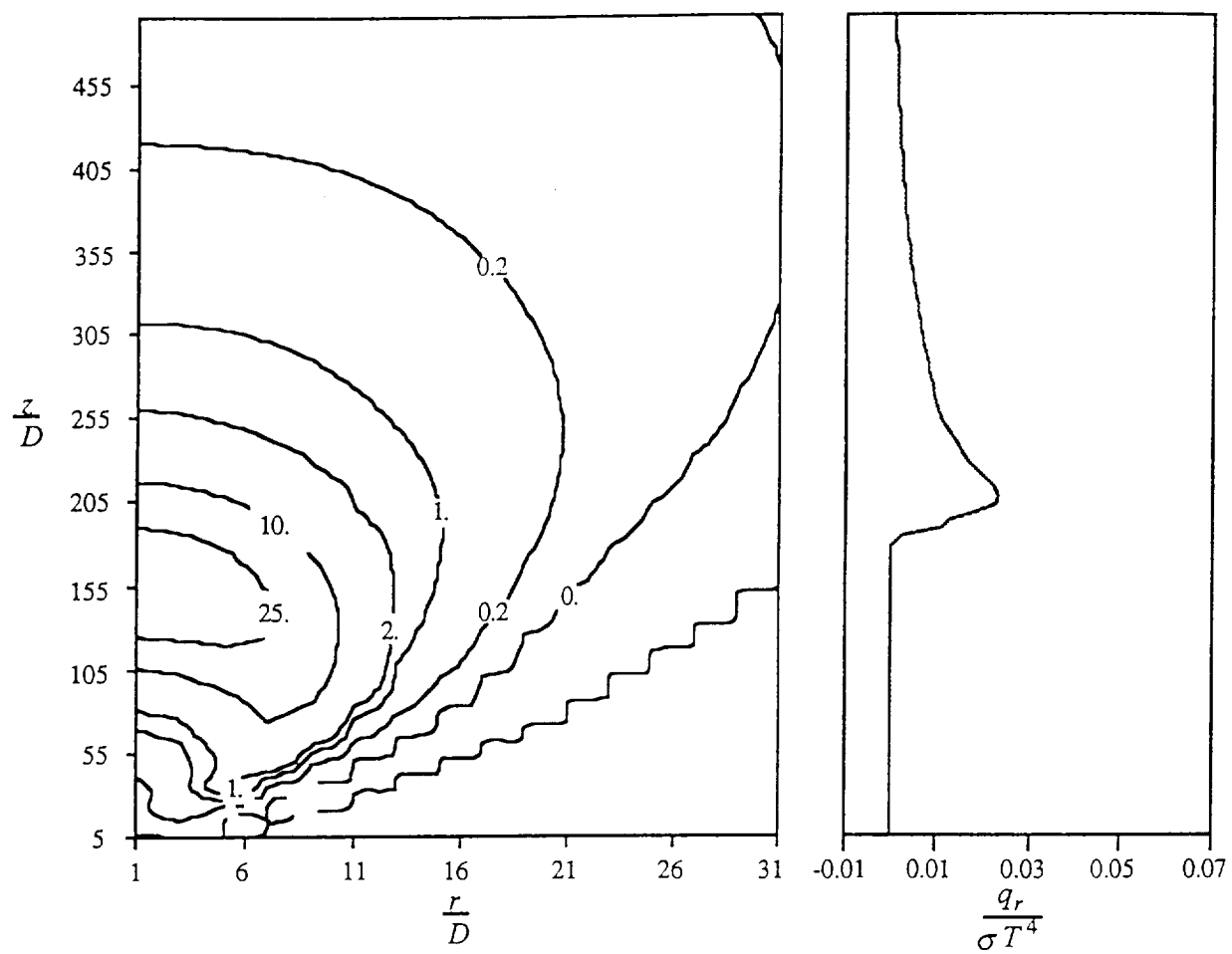


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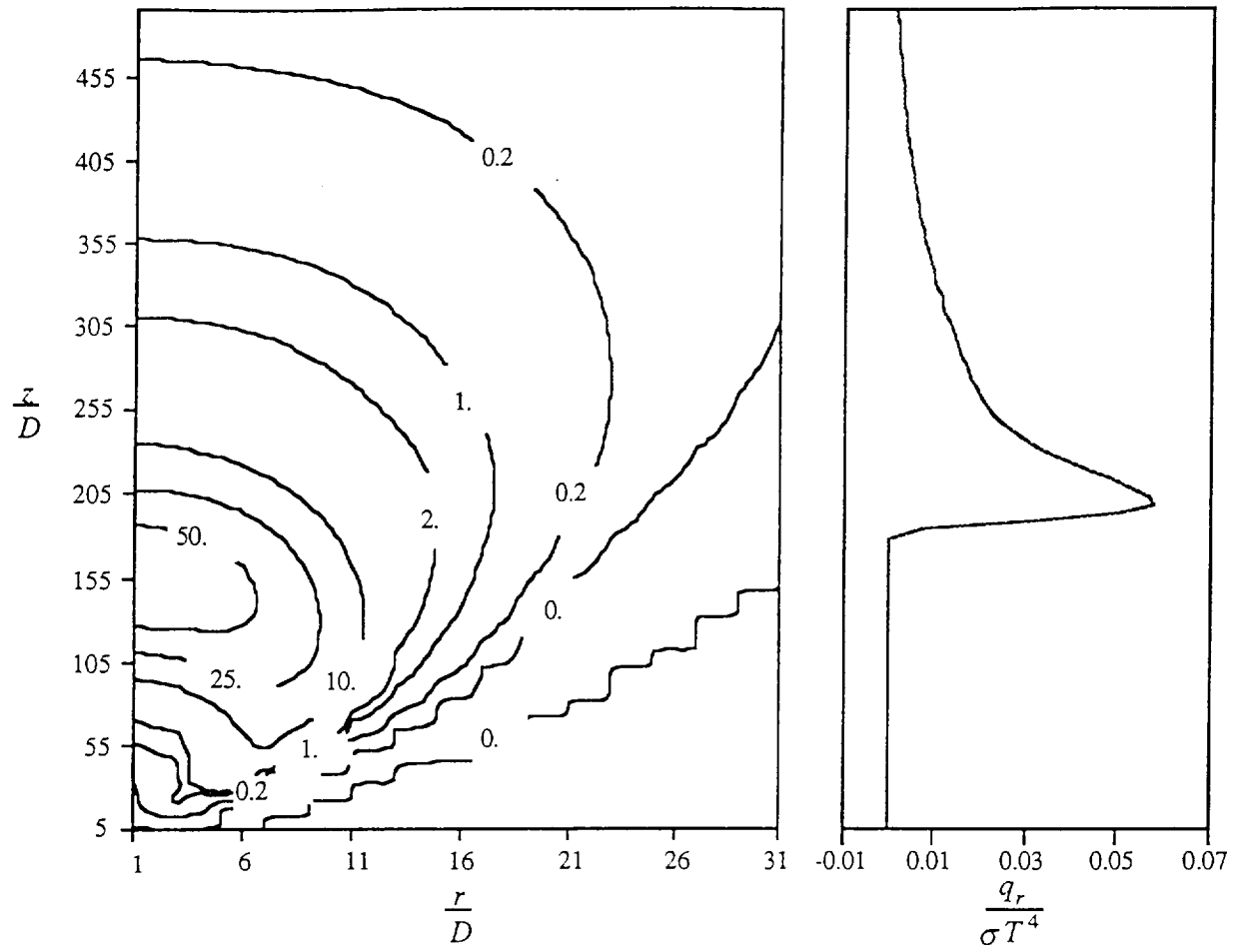


Figure 5

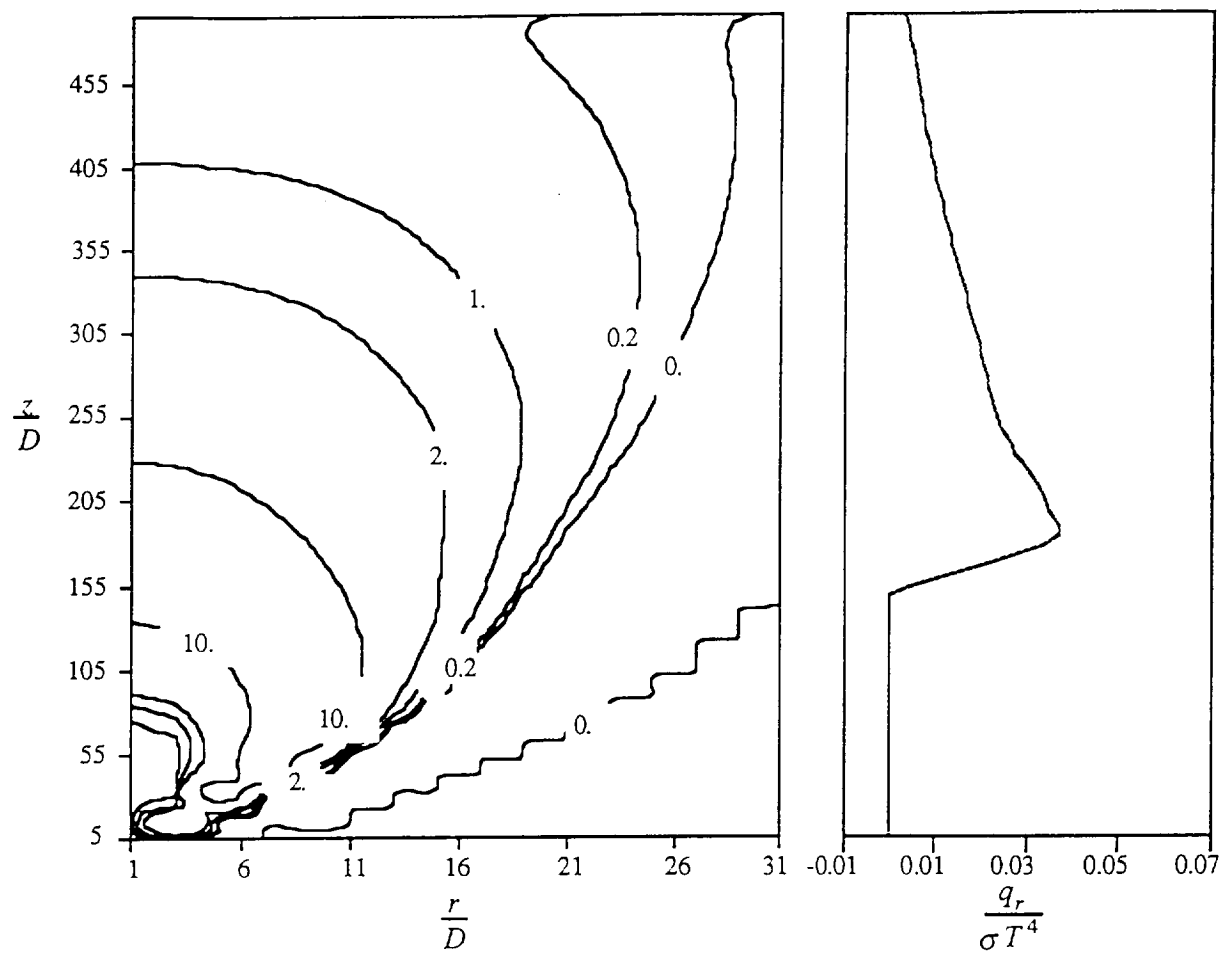


Figure 6

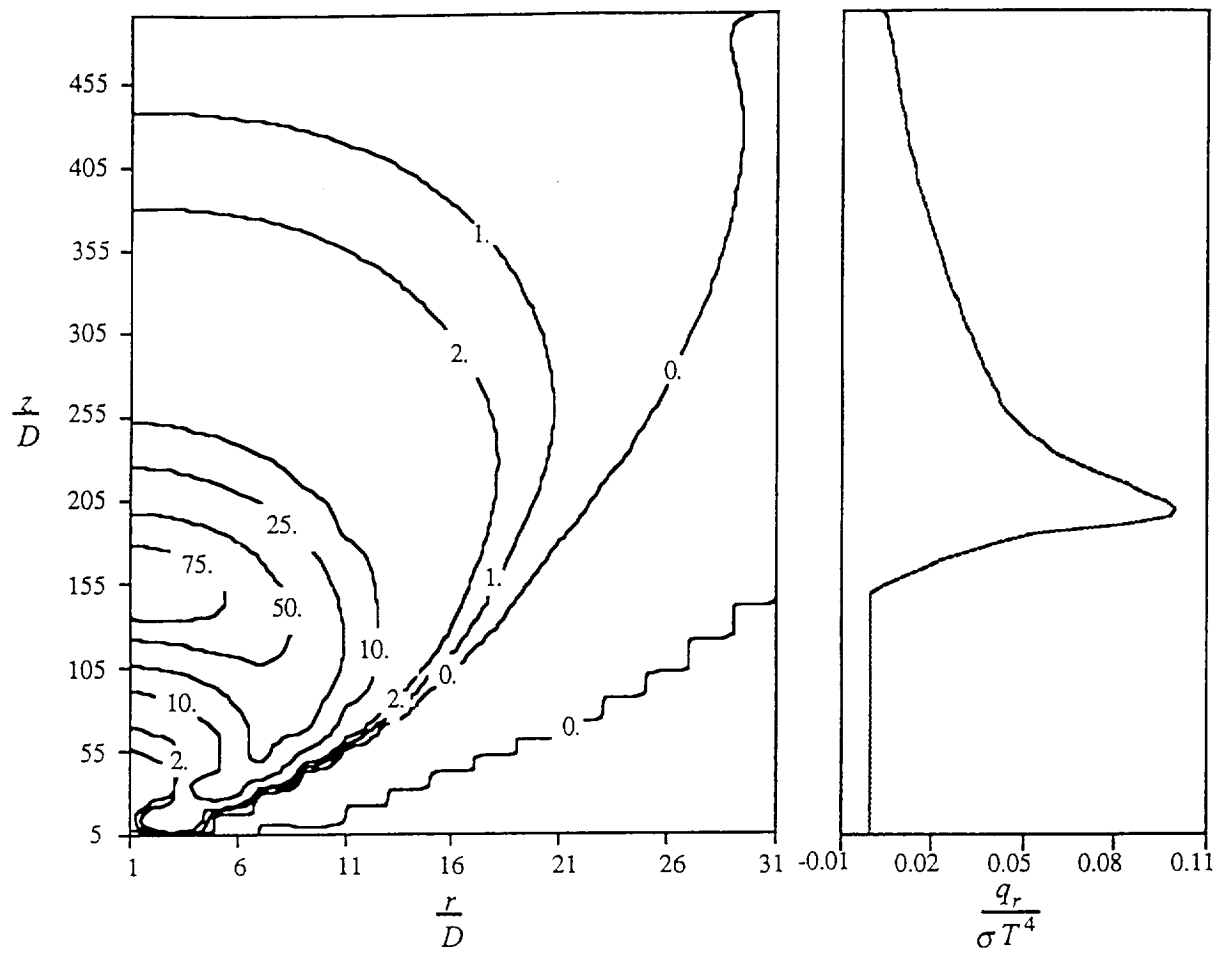


Figure 7

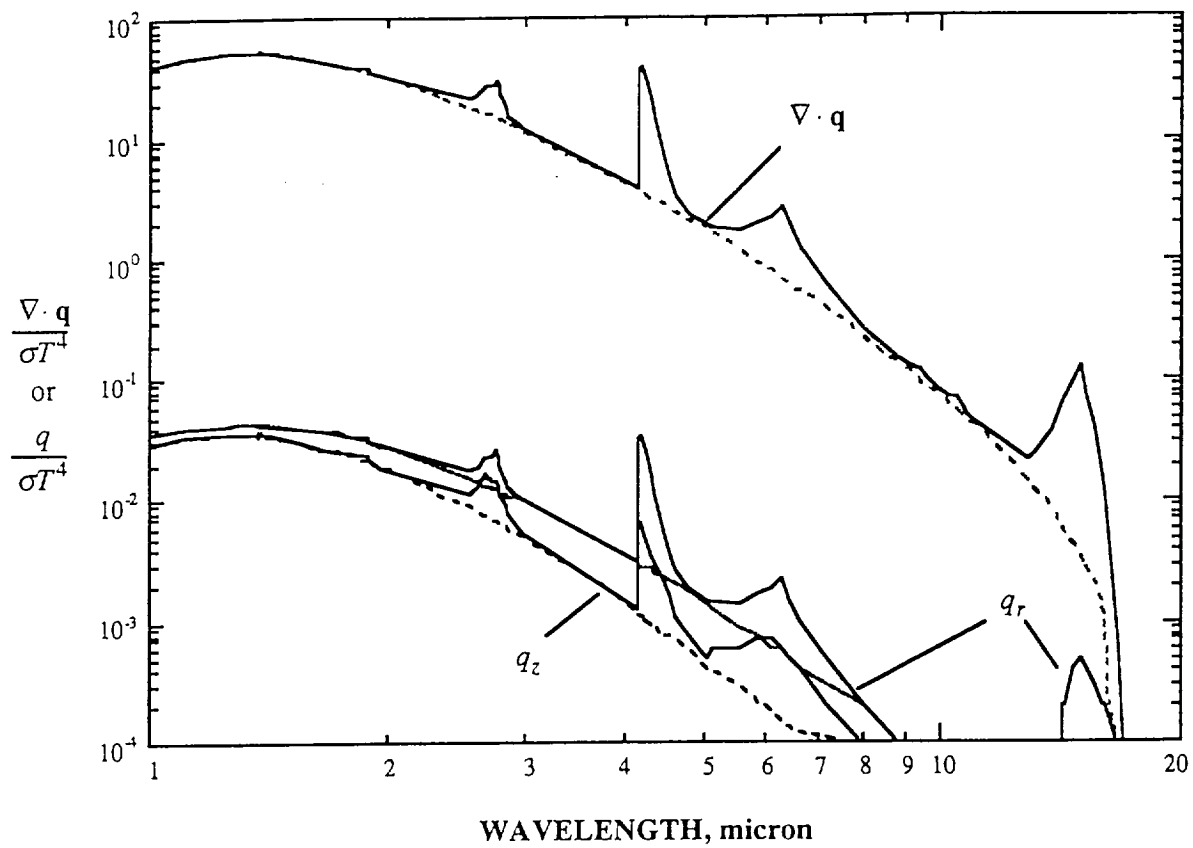


Figure 8